2-Methylphenanthrene

2531-84-2 | DTXSID1025649

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.32e-07 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.68e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

Image not found
Aldrin
Measured: 4.66e-08
Predicted: 9.23e-08

Image not found
Chlordane
Measured: 1.37e-07
Predicted: 1.30e-07

Image not found
cis-Chlordane
Measured: 1.37e-07
Predicted: 1.30e-07

Image not found
trans-Chlordane
Measured: 1.37e-07
Predicted: 1.30e-07

Image not found
Naphthalene, 1-iodo-
Measured: 2.82e-05
Predicted: 1.16e-05

Image not found
Dienochlor
Measured: 5.27e-08
Predicted: 8.74e-08

Image not found
Heptachlor
Measured: 4.82e-07
Predicted: 3.17e-07